Detailed atomic, molecular and radiation kinetics in current 2D and 3D edge plasma fluid codes

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OUTLINE: A&M Model in EIRENE, B2-EIRENE, EMC3-EIRENE, OSM-EIRENE, EDGE2D-EIRENE
www.eirene.de

1) A&M effects on ITER divertor predictions
2) A&M effects for divertor data interpretation
3) New databases: status
4) Radiation transport: status
5) Conclusions/Outlook

Consistent Plasma-Gas-Radiation simulations (B2-EIRENE)

If the plasma is allowed to react self-consistently on modified gas-radiation properties, it does so (for ITER conditions) by an increased divertor plasma density, (up to factor 2), somewhat lowered plasma temperature, and a shift from a target recycling towards a volume recombination regime.

This is opposite to expectations for simple estimates that radiation trapping should reduce volume recombination [4,5].

Dominant recombination channels are threebody and radiative. MAR negligible in divertors [2]. Opposite finding, with same numerical model, for linear devices [3]

Motivation

Atomic and molecular reactions in **B2-EIRENE 1996 (and SOLPS 5)**:
- ionisation of atoms, charge-exchange (*D*) and elastic (*He*) collisions
- 3-body and radiative recombination of D^+
- electron-molecule collisions: $D_2 \rightarrow 2D; D_2 \rightarrow D_2^+; D_2 \rightarrow D^+ + D$
- electron-molecular ion collisions: $D_2^+ \rightarrow 2D; D_2^+ \rightarrow D^+ + D; D_2^+ \rightarrow 2D^+$

Update in **B2-EIRENE 2003-2004**:
- Neutral - Neutral collisions between D, D_2, He
- Molecule - Ion elastic collisions ($D_2 + D^+$)

} Viscosity

- Effective rates for electron collisions with D_2 and D_2^+
- Molecular Activated Recombination $D_2(\nu) + D^+ \rightarrow D + D_2^+,\ D_2^+ \rightarrow 2D$

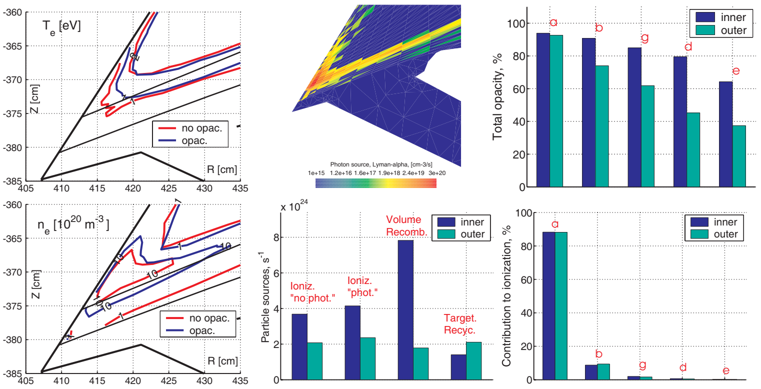
} Molecular Kinetics

Update in **B2-EIRENE 2005**
- Trapping (opacity) of Ly - series photons
- Ionisation of the photoexcited states

} Photon trapping

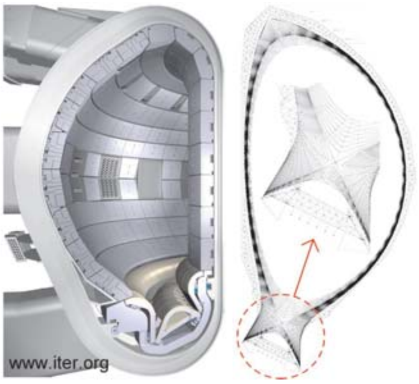
Effect of Photon Trapping

Principal effect: higher density and lower temperature near the targets



Cases with $D_{puff} = 1.5 * 10^{23}\ s^{-1}$ with (P_{PFR} = 10.5 *Pa*) and without (11.3 *Pa*) opacity.

B2-EIRENE



ITER design Computational grid

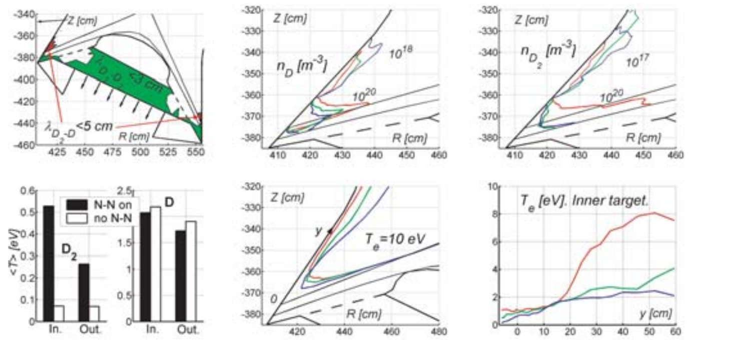
Simulation of the steady state divertor (SOL) conditions for D-He-C plasma.

B2. 2D, time-dependent set of fluid (Braginskii) equations.
EIRENE. Monte-Carlo neutral transport. Calculates neutral related particle, momentum and energy sources for B2.

The goal of the modelling for ITER: *quantitative* assessment of the principal operational parameters (impurity concentration, loads) vs. control parameters (puffing/pumping, gas pressure)

Effect of Viscosity

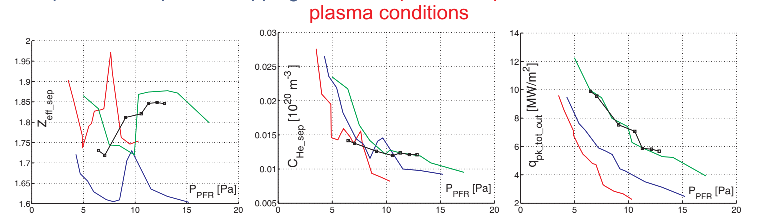
Principal effect: heating of molecules and reduction of their density



EIRENE 1996 $\left(q_{pk\_in} = 2.7 \frac{MW}{m^2}\right)$; + NNC $\left(2.9 \frac{MW}{m^2}\right)$; + D_2 viscosity & kinetics $\left(3.3 \frac{MW}{m^2}\right)$;

ITER operational parameters

Principal effect of viscosity: shift of operational window towards higher pressure
Principal effect of photon trapping: none on operational parameters, but different plasma conditions



EIRENE 1996; + NNC; + D2 viscosity & kinetics; + photon trapping

Application on fixed (reconstructed) plasma background

Sensitivity at low temperature conditions to atomic and molecular physics details.
Strong sensitivity to radiation opacity assumptions

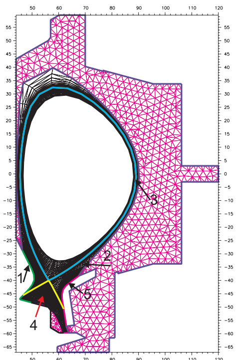
(same as observed in ITER case for frozen plasma conditions)

Inferred atoms density (and related line radiation) differs by factor 2 from opt. thin assumption. This confirms first predictions [6] and is not in conflict with the much lower sensitivity on neutral gas pressure found in self consistent B2-EIRENE ITER calculations.

Results

Geometry and plasma background

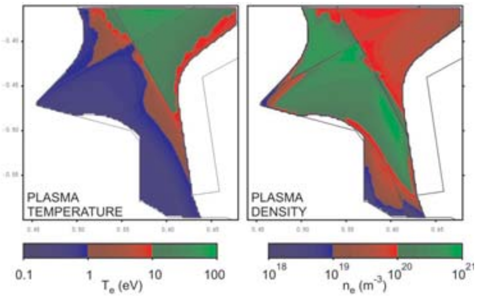
The present study is carried out for operating conditions typical of the compact tokamak device Alcator-C-Mod [5,8].



The plasma parameters, T_e, n_e, are set from comparisons with probe and spectroscopic measurements using the OSM Code [8].

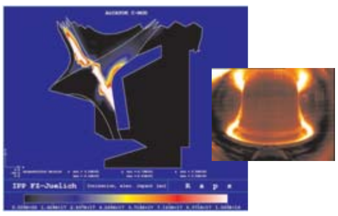
The electron density in PFR is around 10^{21} m^{-3}. The electron temperature there is ~0.5eV and increases towards the outer divertor target.

2D-schematic view of a poloidal cross section of the C-Mod vessel (torus) with a computational grid applied for EIRENE: 1-inner divertor target; 2-scrape-off layer (SOL); 3-separatrix; 4-private flux region (PFR); 5- outer divertor target.

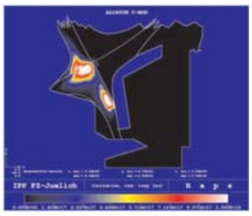


Divertor plasma solution from OSM-code.

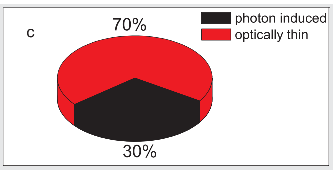
Ionization sources



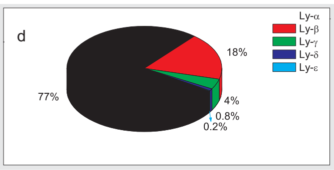
a) ordinary re-ionization source



b) extra re-ionization source due to photon absorption



c) contribution of photon trapping to the total ionization source.



d) contribution of the individual lines to the photon-induced ionization.

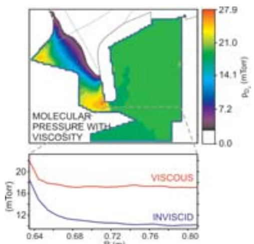
Same figure for JET: 85-15
Same figure for ITER: 30-70

Neutral Pressure

Exp:	25 mTorr
Calc 2D (2000)	3 mTorr
Calc 2D (2003)	27 mTorr [8]

(better A&M data, better Plasma data)

However
Ly-opacity: 17 mTorr
3D: 11 mTorr

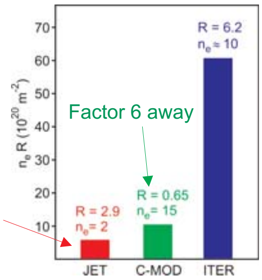


Current hypothesis:
in the "detached state" is the divertor dynamics and chemistry is controlled by "Collisionality"

(inv. Knudsen number)

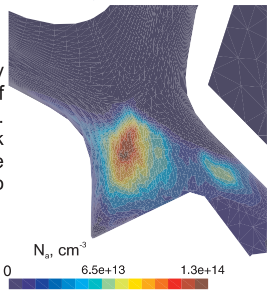
Estimate "Collisionality": $n_e R$
- n_e-Divertor Plasma density (×10^{20} m^{-3})
- R- Major Radius (m)

Alcator C-Mod (MIT)
10 times smaller than ITER
similar shape
Higher density

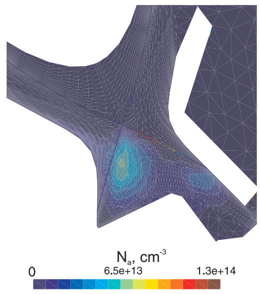


Atomic and photon density

The atomic density reaches peak values of ~10^{14} cm^{-3} in the PFR. Another smaller peak near the outer leg of the separatrix is also pronounced.



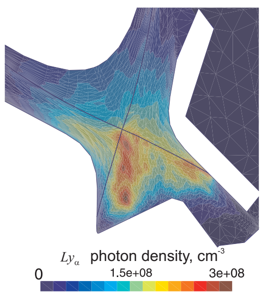
Atomic density (without photon absorption)

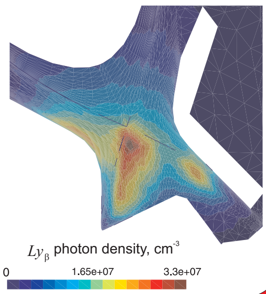


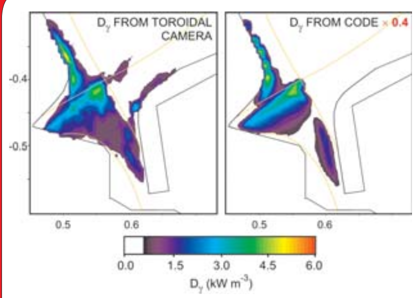
Atomic density with photon absorption (compare with

When accounting for absorption, the calculated atom density drops significantly

Ly-photons generated by the five transitions Ly-α to Ly-ε are considered. The atoms, after absorption, can be ionized before re-emission of photons or suffer collisional decay.







D_γ (from D, D_2, D^+, D_2^+):
Profile matched, but high by factor 2
Calibration? Atomic Data? Plasma reconstruction?

Results very sensitive eg. to T_e profile

Model validation in the presence of many free parameters:

include ALL edge physics that we are sure must be operative even while our capability to confirm these directly remains limited

New Hydride Collision Databases for Technical Plasmas and Fusion Plasmas

Databases used in (fusion) applications are sometimes either entirely obsolete, or, at best, incomplete and largely empirical

Reviewed cross section σ(E) Database Series 2002-2003, FZ-Jülich, NIFS (Japan), IAEA (R. Janev et al.)

Methane (CH_y) C_2H_y C_3H_y Silane (SiH_y)

JUEL 3966, Feb 2002 Phys. Plasmas, Vol 9, 9, (2002) 4071

JUEL 4005, Oct. 2002 Phys. Plasmas, Vol 11,2, (2004) 780

JUEL 4038, Mar. 2003 Contr. Plas.Phys, 47, 7, (2003) 401-417

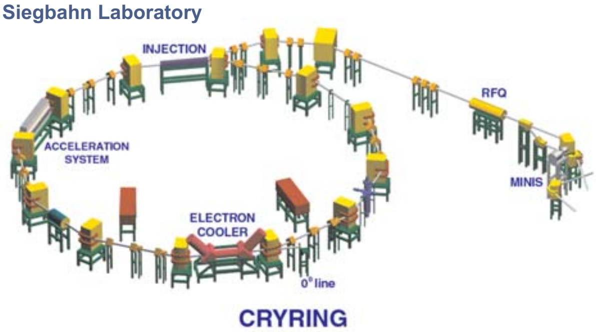
IAEA-TCM 2005-2008: verification and new results (exp. + theor.)

Table 1
Branching ratios of the dissociative recombination of $C_3H_4^+$

Reaction pathway	Products	Branching ratio	Janev & Reiter
1a	$C_3H_3 + H$	0.87 ± 0.04	0.30
1b	$C_3H_2 + H_2$	≤0.02	
1c	$C_2H_3 + CH$	0.01 ± 0.01	
1d	$C_2H_2 + CH_2$	0.06 ± 0.02	
1e	$C_2H + CH_3$	0.01 ± 0.01	
1f	$C_3H_2 + 2H$	≤0.05	0.55

Int. J. Mass Spectrom. **237**, 25 (2004) (Mats Larsson)

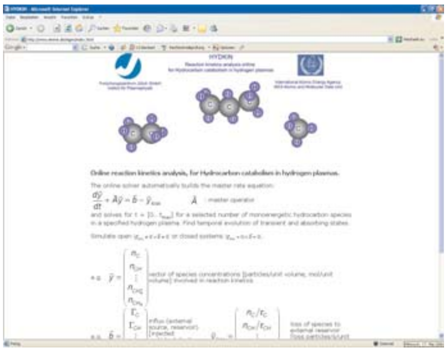
Manne Siegbahn Laboratory

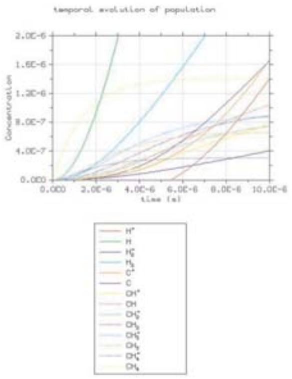


52 meters circumference

Analysis tool for hydrocarbon catabolism in fusion edge plasmas

Online evaluation of cross sections σ(E), rate coefficients K(T), rate equations and S/XB, based upon recent database (2004)
www.eirene.de/eigen/index.html

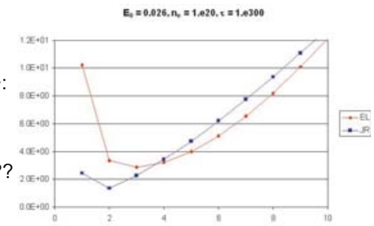




Online solution of time-dep. (1D) Hydrocarbon brake-up, for any prescribed divertor plasma conditions, up to C_3H_8

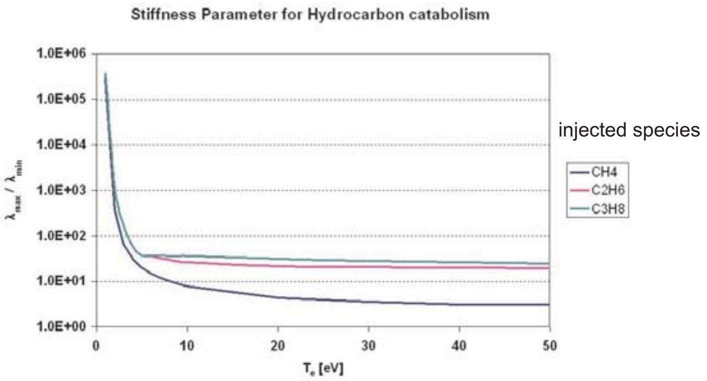
S/XB, compare: Ehrhardt-Langer (EL) - Janev-Reiter (JR)

- S/XB values (photon-efficiencies) for interpretation of CH, C2 band emission
- S/XB =[Influx_C_xH_y /n_CH] /<ex>
- First factor from HYDKIN online tool <ex>: excitation rate coefficient
  - 3 major remaining uncertainties:
  - Born-Bethe approximation for <ex> ??
  - other processes populating upper state??
  - spectral range and v-v Band contributions ??



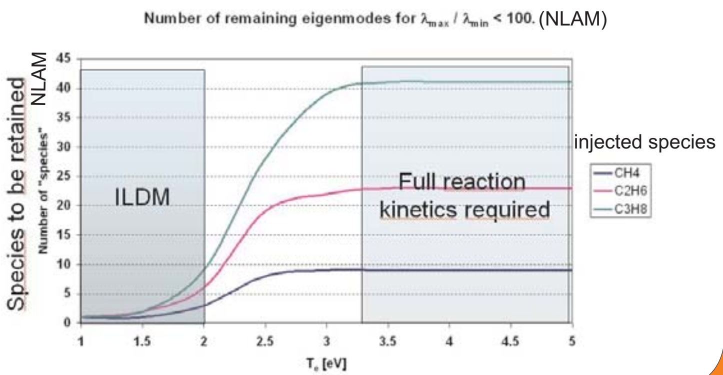
Very complex reaction chains (approx. 500 individual processes) in fusion plasmas: catabolic sequence dominant, little anabolism
- Eigenmode analysis of reaction rate equations very simple:
- Define "Stiffness parameter": $\lambda_{max}/\lambda_{min}$, ratio of max. to min. eigenvalues

Fast slow



Combustion and flame modelling is mathematically analog to diffusion-reaction modelling of ITER divertor detachment.

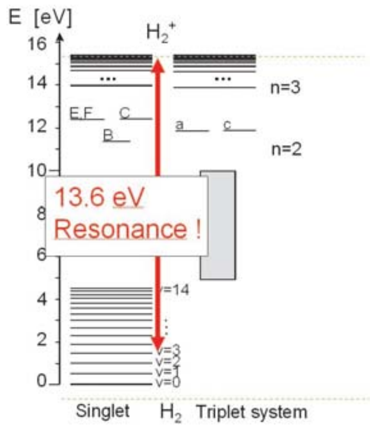
Unfortunately: reduced models („intrinsic low dimensional manifolds, ILDM") only applicable at very low plasma temperatures



New Hydrogen Collision Database fot Technical Plasmas and Fusion Plasmas

H_2 molecule, status in present divertor code

compiled 1997 [7]



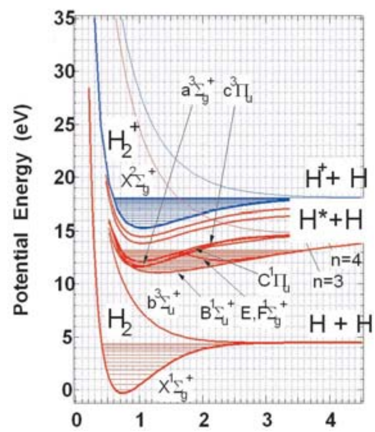
2006-2007 ? New compilation: Janev/Reiter/Samm

p,H,H⁻,H_2,H_2^+,H_3^+

JUEL 4105, Dec. 2003
Encycl. Low. Temp. Pl.
2006, in printing, (in Russian)

More complete models available, still need to be integrated

compiled 2005 [K. Sawada, priv. comm.]



now added: completely v-v' resolved cross sections X->B,C by impact parameter methode calculations (R. Celiberto, Univ. Bary)

Transport of photons

Monte-Carlo transport of photons in EIRENE [6].

1) Sampling of direction of emission
2) Sampling of Zeemann component
3) Sampling of Natural broadening of component plus Doppler shift:

$$E_m = E_0 + m \cdot \mu_B B, \quad P(m) = \frac{1}{4}\begin{cases} 1+\cos^2\Theta, m = \pm 1; \\ 2\sin^2\Theta, m = 0 \end{cases}, \quad \cos\Theta = \frac{v_{ph} B}{cB}$$

$$E = E'\left(1 + \frac{v_{ph} \cdot v_n}{c^2}\right), \quad f(E') = \frac{1}{\pi}\frac{\gamma}{(E' - E_m)^2 + \gamma^2}, \quad \gamma = \frac{A_{n1} h}{4\pi}$$

Absorption cross section (Convolution Integral for Doppler broadening):

$$\sigma_a(E) = \frac{B_{1n} E_0}{\sqrt{\pi}\, c \Delta_D} \sum_{m=-1,0,1} \left(\mathrm{Re}\left[W\left(\frac{E - E_m}{\Delta_D}; \frac{\gamma}{\Delta_D} \right) \right] P(m) \right) \qquad E_m = E_0 \left(1 + \frac{v_{ph} \cdot u}{c^2} \right) + m \cdot \mu_B B,$$

$$\Delta_D = \frac{E_0}{c}\sqrt{\frac{2T}{m_a}} \qquad W(x,y) = W(z = ix - y) = e^{z^2} \cdot \left[1 - \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt \right] \text{ (Faddeeva function)}$$

Collision-radiative model

Sawada-Fujimoto model [7] supplemented with photo-excitation sources:

$$\left(\left[\sum_{q>p} C_{p\to q} + \sum_{q<p} F_{p\to q} + S_p \right] \cdot n_e + \sum_{q<p} A_{p\to q} \right) \cdot n_p - \sum_{q<p} C_{q\to p} n_e n_q - \sum_{q>p} F_{q\to p} n_e n_q - \sum_{q>p} A_{q\to p} n_q =$$

$$= \underbrace{R_p n_e n_+}_{\text{Population } n_p^+} + \underbrace{\left(C_{1\to p} n_e + B_{1\to p} n_{ph}^{1p} \right) \cdot n_1}_{\text{Population } n_p^1}$$

Where C: electronic excitation; F: electronic de-excitation; A: spontaneous transition; S: ionization; R: recombination; B: photo-excitation.

Effective ionization rate $\left(r_p = n_p^1 / n_1 \approx n_p^1 / n_0 \right)$:

$$S^{ph} = \sum_p S_p r_p = S_1 + \sum_{p>1} \left[\left(B_{1p} r_p n_{ph}^p + C_{1p} \right) - \left(F_{p1} + A_{p1}/n_e \right) r_p \right]$$

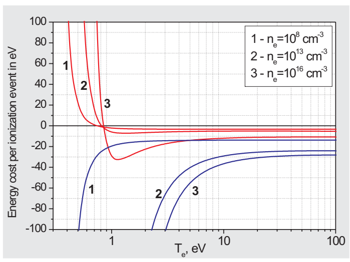
Effective electron cooling rate:

$$S_E^{ph} = S_1 E_0 + \sum_{p>1} S_p \Delta E'_p r_p + \sum_{p>1} C_{1p} \Delta E_{1p} + \sum_{p>1}\sum_{q>p} C_{pq} \Delta E_{pq} r_p - \sum_{p>1}\sum_{q<p} F_{pq} \Delta E_{pq} r_p =$$

$$= S_1 E_0 + \sum_{p>1}\sum_{q<p} A_{pq} \Delta E_{pq} r_p - \sum_{p>1} B_{1q} n_{ph}^{1p} \Delta E_{1p}; \quad \Delta E'_p = E_0 - E_p, \quad \Delta E_{pq} = \left| E_p - E_q \right|$$

Radiative heat transfer into PFZ

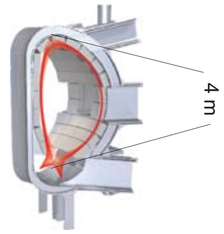
In the case of *Ly* -alpha absorption stimulated ionization the values of the energy cost per one ionization event are positive for T_e below 1 *eV*, i.e. electrons re-gain energy through this ionization channel, via the radiation field. This effect can result in radiative heat transfer from hotter to colder regions even in divertor plasmas.



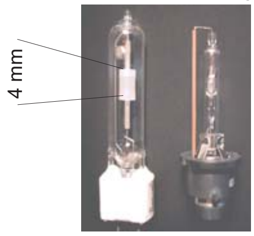
Effective energy source per one ionization event: in blue: ordinary ionization, in red: photon absorption stimulated ionization

Radiation transfer module: verification and validation using HID lamps

ITER



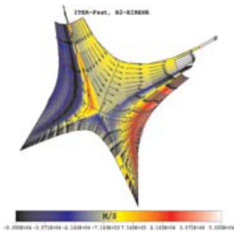
High Intensity Discharge Lamps



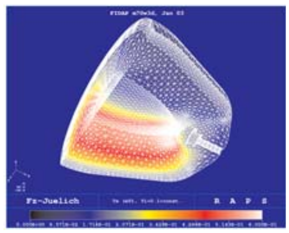
D2-36 W
Automotive
Material:Quartz

CDM-75 W
Shop-Lighting
Material:PCA

B2-EIRENE



FIDAP-EIRENE



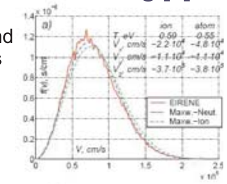
Velocity-space effects (differences to Cretin-Beline modelling [9]

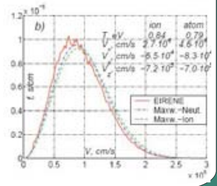
Instead of photo-induced ionization one can use ionization and recombination rates with suppressed spontaneous transitions Both approaches are equivalent in terms of particle balance, but not equivalent in terms of kinetic equation:

Continuity equiation	Boltzmann equation
$\frac{1}{n_e}\left(\frac{dn_0}{dt}\right)_{i/r} = Rn_+ - Sn_0$	$\frac{1}{n_e}\left(\frac{df_0}{dt}\right)_{i/r} = Rn_+ \hat{f}_+ - Sn_0 \hat{f}_0$

S and *R* are effective ionization and recombination rates.

How much is the difference between $\hat{f}_+$ and $\hat{f}_0$? An example of Velocity Distribution function for D atoms on separatrix in front of the inner (a) and outer (b) target →





Emission and absorption line shape profiles in EIRENE (2006)

0) monoenergetic (delta-function, ohne for emission
1) 0 + Doppler (Gaussian profile)
2) Natural broadening, electr. Stark effect (Lorentz-profile)
3) 2 + Doppler (Voigt-profile)
4) Pressure broadening: v.d. Waals, resonance broadening, quadr. Stark (complex Fadeeva function)
5) Not in use
6) Normal Zeeman triplet, (3 monoenergetic components, anisotropic)
7) 6 + Doppler (3 gaussian components, anisotropic)
8) Normal Zeeman triplet, (3 Lorentzian components, anisotropic)
9) 8 + Doppler (weighted sum of 3 Voigt profiles, anisotropic)
10) Full Zeeman-Stark quantal line shape calculation (Rosato et al., Univ. Marseille) (weighted sum of 10 Lorentzian profiles, anisotropic)
11) 10 + Doppler (weighted sum of 10 Voigt profiles, anisotropic)

4): for code verification using HID lamp spectroscopy, LTE, industrial applications (FIDAP-EIRENE)
9): current EIRENE default in B2-EIRENE, OSM-EIRENE, EMC3-EIRENE
10,11): new options (2006), under evaluation

Conclusions/Outlook

- Radiation transfer included also in self consistent 2D plasma-gas-radiation code (B2-EIRENE_ITER) Complementary results in interpretative and predictive mode
- Hydrocarbons: online analysis tool HYDKIN: (www.eirene.de/eigen/index.html) spectral analysis indicates: no reduced models above 3-5 eV ??

References

See also:
[1] A. Kukushkin et al., this conf.
[2] V. Kotov et al., Contrib. Plasmas Physics 2006, in printing
[3] M. Baeva et al., this conf.
[4] D. Reiter, S. Wiesen, M. Born, Plasma Phys. Control. Fusion 44 (2002), 1723.
[5] J. L. Terry, B. Lipschultz, A. Yu. Pigarov et al., Phys. Plasmas 5 (1998), 1759.
[6] D. Reiter, S. Wiesen, M. Born, J. Nuclear Materials, vol. 313-316 (2003), p. 845
[7] K. Sawada, T. Fujimoto, J. Appl. Phys. 78 (1995) 2913.
[8] S. Lisgo, P. Börner, C. Boswell et al., J. Nucl. Mat. 337-339 (2005), 139.
[9] H.A. Scott, M.L. Adams, Contrib. Plasma Phys, 44, 51(2004) and M.L. Adams, H.A. Scott, Contrib. Plasma Phys, 44, 262 (2004)